

4,5-Dibromo-1-methyl-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)-1H-pyrrole-2-carboxamide
113589-14-3 | DTXSID20556731

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.35 days

Global applicability domain: Outside

Local applicability domain index: 3.08e-01

Confidence level: 9.19e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Methyl-2-propylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.17</div>	<div>Image not found</div> <div>3-Ethyltoluene</div> <div>Measured: 12.5</div> <div>Predicted: 3.26</div>	<div>Image not found</div> <div>1,3-Dimethyl-4-ethylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 3.89</div>
<div>Image not found</div> <div>2-Ethyl-p-xylene</div> <div>Measured: 12.5</div> <div>Predicted: 3.70</div>	<div>Image not found</div> <div>1-Ethyl-2-methylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 3.88</div>	